END

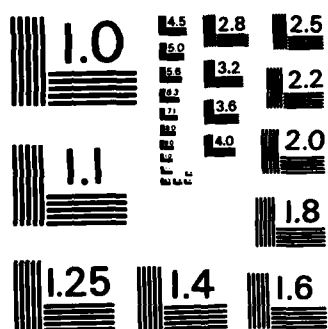FILMED

DTIC
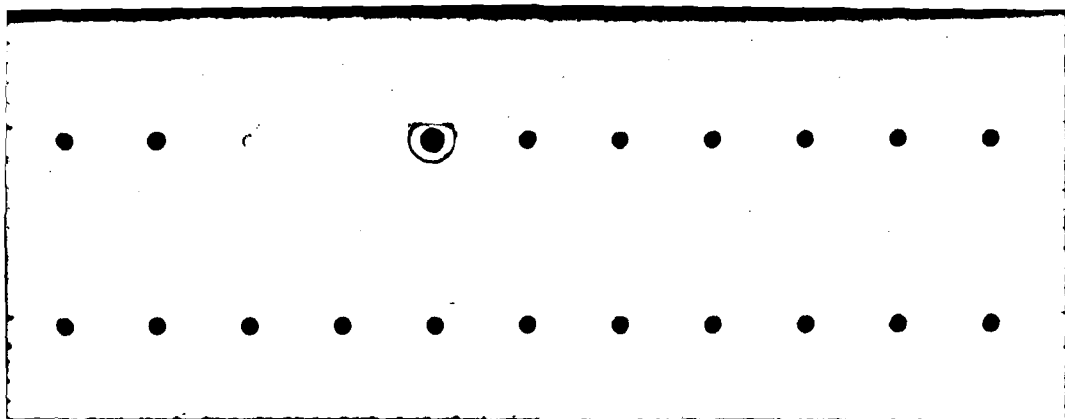
MICROCOPY RESOLUTION TEST CHART

NATIONAL BUREAU OF STANDARDS-1963-A

4

OPTIMAL INCOMPLETE BLOCK DESIGNS

FOR COMPARING TREATMENTS WITH A CONTROL

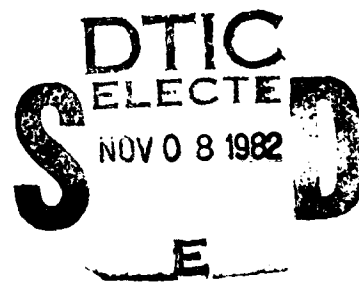by

Dibyen Majumdar[1], University of Illinois at Chicago Circle

and

William I. Notz, Purdue University

July 1982

DTIC
ELECTE
NOV 0 8 1982
S   D
E

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER AFOSR-TR- 82-0953	2. GOVT ACCESSION NO. AD-A121 184	3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle) OPTIMAL INCOMPLETE BLOCK DESIGNS FOR COMPARING TREATMENTS WITH A CONTROL	5. TYPE OF REPORT & PERIOD COVERED TECHNICAL
	6. PERFORMING ORG. REPORT NUMBER

7. AUTHOR(s) William I. Notz, Purdue University, and A.S. Hedayat, University of Illinois at Chicago Circle	8. CONTRACT OR GRANT NUMBER(s) AFOSR-80-0170

9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Mathematics, University of Illinois at Chicago Circle, Box 4348, Chicago IL 60680	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS PE61102F; 2304/A5

11. CONTROLLING OFFICE NAME AND ADDRESS Directorate of Mathematical & Information Sciences Air Force Office of Scientific Research Bolling AFB DC 20332	12. REPORT DATE July 1982
	13. NUMBER OF PAGES 19

14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)	15. SECURITY CLASS. (of this report) UNCLASSIFIED
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Incomplete block designs; BTIB designs; BIB designs; binary designs; comparing p treatments to a control; ϕ-optimality; D-optimality; A-optimality; E-optimality.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The problem of finding optimal incomplete block designs for comparing p test treatments with a control is studied. BIB designs are found to be D-optimal. A- and E-optimal designs are also obtained. For a large class of functions ϕ, conditions for a design to be ϕ-optimal are found. Most of the optimal designs are certain types of BTIB designs (introduced by Bechhofer and Tamhane (1981)) which are binary in test treatments.

DD FORM 1473 EDITION OF 1 NOV 65 IS OBSOLETE

82 11 08 043

ABSTRACT

The problem of finding optimal incomplete block designs for compar-
ing p test treatments with a control is studied. B.I.B. designs are
found to be D-optimal. A- and E-optimal designs are also obtained.
For a large class of functions ϕ, conditions for a design to be ϕ-optimal
are found. Most of the optimal designs are certain types of B.T.I.B. de-
signs (introduced by Bechhofer and Tamhane (1981)) which are binary in
test treatments.

Keywords and phrases: Incomplete block designs, BTIB designs, BIB de-
signs, binary designs, comparing p treatments to a control, ϕ-optimality,
D-optimality, A-optimality, E-optimality.

AMS 1970 Classification: Primary 62K05; Secondary 62K10

1. Introduction

Consider an experimental situation where it is desired to compare $p \geq 2$ test treatments to a control treatment. Let the $p + 1$ treatments be indexed $0, 1, \ldots, p$ with 0 denoting the control treatment and $1, 2, \ldots, p$ denoting the test treatments. It is desired to compare simultaneously the p test treatments to the control. For improving the precision of the comparisons the experimental units are to be blocked in b blocks each of size k, $2 \leq k \leq p$. We are then in an incomplete block design setting.

Let Y_{ijh} denote the observation on treatment $i(0 \leq i \leq p)$ in block $j(1 \leq j \leq b)$ in plot $h(1 \leq h \leq k)$. We assume the usual additive linear model without interactions, namely

$$(1.1) \qquad Y_{ijh} = \mu + \alpha_i + \beta_j + \varepsilon_{ijh},$$

the ε_{ijh} are assumed to be uncorrelated random variables with mean 0 and common variance σ^2. The p control-treatment contrasts $\alpha_0 - \alpha_i$ are to be estimated by their BLUEs $\hat{\alpha}_0 - \hat{\alpha}_i$ $(1 \leq i \leq p)$. It is desired to choose an experimental design (an allocation of treatments to blocks) which will yield the best, in some sense, set of estimates among all possible designs.

For given values of b, k, and p let $C(b,k,p)$ denote the class of all possible incomplete block designs with b blocks, each of size $k(p \geq k \geq 2)$, p test treatments indexed $1, \ldots, p$, and a control treatment indexed 0. For a design $d \in C(b,k,p)$ let $r_{ij}(d)$ denote the number of replications of treatment $i(0 \leq i \leq p)$ in block $j(1 \leq j \leq b)$. Also let $r_i(d) = \sum\limits_{j=1}^{b} r_{ij}(d)$ and $\lambda_{i\ell}(d) = \sum\limits_{j=1}^{b} r_{ij}(d) r_{\ell j}(d)$ $(0 \leq i \neq \ell \leq p)$. Notice $r_i(d)$ represents the number of replications of treatments in the entire design d and $\lambda_{i\ell}(d)$ represents the number of times treatments i and ℓ are paired together in a block summed over all blocks.

For $d \in C(b,k,p)$, let $M(d)$ denote the information matrix corresponding to estimating all $\alpha_0 - \alpha_i$, $1 \leq i \leq p$, (as in Bechhofer and Tamhane (1981)). $M(d)$ is a nonnegative definite $p \times p$ matrix and is nonsingular if and only if all the $\alpha_0 - \alpha_i$ are estimable, in which case it is proportional to the inverse of the covariance matrix of $\hat{\alpha}_0 - \hat{\alpha}_i$, $1 \leq i \leq p$.

We now make our goal of finding a design $d \in C(b,k,p)$ which gives us the best, in some sense, set of BLUEs $\hat{\alpha}_0 - \hat{\alpha}_i (1 \leq \ell \leq p)$ more explicit. Following the work of Kiefer (see for example Kiefer (1958, 1959, 1971, and 1974)) we seek a $d \in C(b,k,p)$ which minimizes $\phi(M(d))$ for some function ϕ over $C(b,k,p)$. Such a design will be called ϕ-optimal. Restricting to non-singular designs, some common examples of ϕ are $\phi_0(M(d)) = \det M^{-1}(d)$ (so called D-optimality), $\phi_1(M(d)) = \operatorname{tr} M^{-1}(d)$ (so called A-optimality), and $\phi_\infty(M(d)) = $ maximum eigenvalue of $M(d)$ (so called E-optimality). In the present context of control-treatment comparisons, A-optimality has an appealing statistical interpretation, viz. it minimizes $\sum_{i=1}^{p} \operatorname{var}(\hat{\alpha}_0 - \hat{\alpha}_i)$ over all designs. We are, however, yet to realize natural statistical interpretations for the other criteria.

Traditionally, Kiefer and other researchers were interested in an orthonormal basis of treatment contrasts. In other words, the aim was to determine good designs for estimating $P\vec{\alpha}$ where $\vec{\alpha}$ is the vector of all the $p + 1$ treatment effects and P is a $p \times p + 1$ matrix of zero row sums and orthonormal rows. Nothing much seems to be known for the situation when the contrasts are not mutually orthogonal. In this paper we look at one such situation - that of control-treatment comparison.

Let $\nu_i(d)$, $1 \leq i \leq p$, be the positive eigenvalues of the well known "C-matrix" of normal equations for $\vec{\alpha}$, for a design d in $p + 1$ treatments in b blocks of k plots each. Let $P\vec{\alpha}$ be any vector of p independent

treatment contrasts, and $V(P\vec{\alpha}(d))$ be the covariance matrix of the BLUE's of $P\vec{\alpha}$. Then it can be shown that

$$\det V(P\vec{\alpha}(d)) = (\det(PP'))(v_1(d)\ldots v_p(d))^{-1}.$$

This can be established by starting from a spectral decomposition of the C-matrix for the design d, or by proving a result like equation (A.2) of Bechhofer and Tamhane (1981). Since a B.I.B. design, if it exists, is D-optimal in the traditional sense of estimating orthonormal contrasts, we have the following theorem.

<u>Theorem 1.1</u> A B.I.B. design, if it exists, is D-optimal for estimating any set of p independent treatment contrasts.

It has come to our notice that this result has been known for some time (Hedayat (1974)). Observe that the D-optimality criterion ignores the particular interests of the experimenter expressed through the matrix P.

From the work of Kiefer and others on optimal incomplete block designs for estimating an orthonormal basis of treatment contrasts, it is known that the B.I.B. design is optimal, not only according to the D-criterion, but under a very large class of optimality criteria as well (see Kiefer (1958, 1959, 1971, 1974 and 1975)). Such results might lead us to expect that in our setting an optimal design d in C(b,k,p) would be symmetric (in some sense) and binary in the test treatments 1,....,p (but not in the control). Since the control plays a special role in our setting we might also expect that the number of replications of the control (more specifically the $r_{0j}(d)$) will be an important factor in determining what design d is optimal. These expectations are indeed found to be the case as will be seen in the results of section 2.

The proper sense of symmetry in a design $d \in C(b,k,p)$ turns out to be that all $\lambda_{i\ell}(d)$ are equal for $1 \leq i \neq \ell \leq p$ and all $\lambda_{0\ell}(d)$ for $1 \leq \ell \leq p$ are equal (but not necessarily to the $\lambda_{i\ell}(d)$ for $1 \leq \ell \leq p$). Such designs are called balanced treatment incomplete block designs (abbreviated BTIBs) and were first introduced in Bechhofer and Tamhane (1981) in connection with making joint confidence statements about the contrasts $\alpha_0 - \alpha_i$, $1 \leq i \leq p$. The interested reader is referred to this paper for more information on BTIB designs. We remark that if a design $d \in C(b,k,p)$ is a BTIB design its information matrix $M(d)$ is completely symmetric (i.e. all off diagonal elements equal and all diagonal elements equal). Bechhofer and Tamhane (1981) also have a review on available literature for designs for control-treatment comparisons.

Section 2 of this paper contains results about what designs are ϕ-optimal for a fairly broad class of functions ϕ. As an important application we discuss A-optimal designs.

The class of functions considered in section 2 does not include E-optimality. This is treated in section 3, which also includes a result showing that an A-optimal design is optimal according to another statistically interesting criterion. Section 4 contains some concluding remarks.

2. A-Optimal Designs

We begin this section with a series of lemmas culminating in a general theorem from which A-optimal designs may be obtained as a special case.

Suppose $d \in C(b,k,p)$ is arbitrary. Let $\natural$ be the set of all $p!$ permutations of the test treatments $1,\ldots,p$. Let $\sigma d, \sigma \in \natural$, be the design resulting from d by the permutation σ of the treatments in d. We define

$$(2.1) \qquad \bar{M}(d) = \sum_{\sigma \in \natural} M(\sigma d)/p! = \sum_{\pi \in \underline{\Pi}} \pi' M(d) \pi / p!$$

where $\underline{\Pi}$ is the set of all $p \times p$ permutation matrices.

Lemma 2.1. If $d \in C(b,k,p)$ then $\bar{M}(d)$ has eigenvalues $\mu_1(d)$, $\mu_2(d) = \ldots = \mu_p(d)$ with

$$\mu_1(d) = \{\sum_{i=1}^{p} \lambda_{0i}(d)/k\}/p = (r_0(d) - \sum_{j=1}^{b} r_{0j}^2(d)/k\}/p$$

$$\mu_2(d) = \{\sum_{i=1}^{p} r_i(d) - \sum_{i=1}^{p} \sum_{j=1}^{b} r_{ij}^2(d)/k - (r_0(d) - \sum_{j=1}^{b} r_{0j}^2(d)/k)/p\}/(p-1).$$

In addition if d is binary in test treatments

$$\mu_2(d) = \{b(k-1) - ((k-1)/k)r_0(d) - (r_0(d) - \sum_{j=1}^{b} r_{0j}^2(d)/k)/p\}/(p-1)$$

pf. From the appendix of Bechhofer and Tamhane (1981), the entries of $M(d)$ are

$$m_{i_1, i_2} = \begin{cases} r_{i_1}(d) - \sum_{j=1}^{b} r_{i_1 j}^2(d)/k & (i_1 = i_2) \\ -\lambda_{i_1 i_2}(d)/k & (i_1 \neq i_2) \end{cases}$$

and the sum of the entries in the i-th row (or i-th column) is $\lambda_{0i}(d)/k$. Thus is it straightforward to check that

$$(2.2) \quad \bar{M}(d) = (\{\sum_{i=1}^{p} r_i(d) - \sum_{i=1}^{p} \sum_{j=1}^{b} r_{ij}^2(d)/k + \sum_{1 \leq i_1 < i_2 \leq p} \lambda_{i_1 i_2}/k(p-1)\}/p)I_p$$

$$- (\sum_{1 \leq i_1 < i_2 \leq p} \lambda_{i_1 i_2}/kp(p-1))J_{p,p}$$

where I_p is the $p \times p$ identity matrix and $J_{p,p}$ is the $p \times p$ matrix all of whose entries are +1. The first part of the lemma now follows from the well known fact that $aI_p + bJ_{p,p}$ has eigenvalues a with multiplicity $p-1$ and $a + bp$ with multiplicity 1. The second part involves essentially straightforward computations only.

Lemma 2.2. Suppose ϕ is a convex real-valued possibly infinite function on the set of all $p \times p$ non-negative definite matrices and ϕ is invariant under permutations, i.e. if π is a permutation matrix, $\phi(\pi'M\pi) = \phi(M)$. Then for $d \in C(b,k,p)$, $\phi(\bar{M}(d)) \leq \phi(M(d))$.

pf. $\phi(M(d)) = \sum_{\sigma \in \natural} \phi(M(\sigma d))/p!$ since ϕ is permutation invariant. Thus by convexity $\phi(M(d)) \geq \phi(\sum_{\sigma \in \natural} M(\sigma d)/p!) = \phi(\bar{M}(d))$.

Lemma 2.3. Suppose ϕ is some real-valued possibly infinite function on the set of all non-negative definite $p \times p$ matrices with the property that if M and N are non-negative definite $p \times p$ matrices with eigenvalues $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_p$ and $\nu_1 \leq \nu_2 \leq \cdots \leq \nu_p$ respectively which satisfy $\mu_i \geq \nu_i$ for $i = 1,\ldots,p$ then $\phi(M) \leq \phi(N)$.

Let $d \in C(b,k,p)$ be a design which is not binary in test treatments. Then there exists $d^* \in C(b,k,p)$ which is binary in test treatments with $r_0(d^*) = r_0(d)$ and which satisties $\phi(\bar{M}(d^*)) \leq \phi(\bar{M}(d))$.

pf. In each block of $M(d)$ replace any duplicates of test treatments by test treatments not in the block so that each block is binary in test treatments (this is possible since $k \leq p$). Call the resulting design d^*. Notice d^* is binary in test treatments, has $r_{0j}(d^*) = r_{0j}(d)$ for all $1 \leq j \leq b$, and has $\sum_{i=1}^{p} r_i(d^*) = \sum_{i=1}^{p} r_i(d)$. As a result it is easy to see

$$\sum_{i=1}^{p} \sum_{j=1}^{b} r_{ij}^2(d^*) \leq \sum_{i=1}^{p} \sum_{j=1}^{b} r_{ij}^2(d).$$

From lemma 2.1 it then follows that the eigenvalues of $\bar{M}(d)$ and $\bar{M}(d^*)$ satisfy $\mu_1(d) = \mu_1(d^*)$ and $\mu_2(d) = \cdots = \mu_p(d) \leq \mu_2(d^*) = \cdots = \mu_p(d^*)$. Hence by the property of ϕ given in the statement of the lemma, $\phi(\bar{M}(d^*)) \leq \phi(\bar{M}(d))$.

Lemma 2.4. Among all non-negative integers $r_{01}, r_{02}, \ldots, r_{0b}$ satisfying $\sum\limits_{j=1}^{b} r_{0j} = r$, where r is a fixed constant, the value of $\sum\limits_{j=1}^{b} r_{0j}^2$ is minimized by choosing $r - b[r/b]$ of the r_{0j} to have value $[r/b] + 1$ and the remaining $b(1+[r/b]) - r$ of the r_{0j} to have value $[r/b]$. Here $[\cdot]$ denotes the greatest integer function.

pf. This is lemma 2.3 of Cheng and Wu (1980).

Lemma 2.5. Suppose ϕ is as in lemma 2.3. Suppose $d \in C(b,k,p)$ is binary in test treatments and has $r_0(d) > bk/2$. Then there exists $d* \in C(b,k,p)$ which is binary in test treatments, has $r_0(d*) < bk/2$, and satisfies $\phi(\bar{M}(d*)) \leq \phi(\bar{M}(d))$.

pf. Take $d*$ to be the design where in each block of d we replace all test treatments by the control and all of the original replications of the control by differing test treatments not originally in the block. Notice

$$(2.3) \quad r_0(d*) = \sum_{j=1}^{b} r_{0j}(d*) = \sum_{j=1}^{b} (k-r_{0j}(d)) = bk - r_0(d) < bk/2 < r_0(d)$$

$$(2.4) \quad r_0(d*) - \sum_{j=1}^{b} r_{0j}^2(d*)/k = r_0(d) - \sum_{j=1}^{b} r_{0j}^2(d)/k.$$

From (2.4) it follows that if $\mu_1(d)$, $\mu_2(d) = \ldots = \mu_p(d)$ and $\mu_1(d*)$, $\mu_2(d*) = \ldots = \mu_p(d*)$ are the eigenvalues of $\bar{M}(d)$ and $\bar{M}(d*)$, respectively, as given in lemma 2.1, then $\mu_1(d) = \mu_1(d*)$. Also from (2.3), (2.4), and lemma 2.1, $\mu_2(d) < \mu_2(d*)$. By the property of ϕ given in the lemma it follows that $\phi(\bar{M}(d*)) \leq \phi(\bar{M}(d))$.

Theorem 2.1. Suppose ϕ is a real-valued possibly infinite function on the set of all $p \times p$ non-negative definite matrices satisfying

$$\phi(M) = \sum_{i=1}^{p} f(\mu_i)$$

where $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_p$ are the eigenvalues of M, f is a real valued possibly infinite function on the set of all non-negative numbers which is continuous on the set of all positive numbers, has $f' < 0$ and $f'' > 0$ (here primes denote differentiation). Suppose there is a $\delta \in C(b,k,p)$ such that $M(\delta)$ is completely symmetric and

(i) δ is binary in test treatments

(ii) $r_0(\delta)$ is the value of the integer r, $0 \leq r \leq [bk/2]$, which minimizes

(2.5) $g(r;b,k,p) = f((r-h(r;b)/k)/p)$

$$+ (p-1)f((b(k-1)-((k-1)/k)r-(r-h(r;b)/k)/p)/(p-1))$$

where

(2.6) $h(r;b) = (b(1+[r/b])-r)[r/b]^2 + (r-b[r/b])([r/b]+1)^2$

(iii) the $r_{0j}(\delta)$ have value either $[r_0(\delta)/b]$ or $[r_0(\delta)/b] + 1$. Then δ is ϕ-optimal over $C(b,k,p)$.

pf. First we notice ϕ and f have the following properties

(a) ϕ is convex and orthogonal invariant (i.e. if π is an orthogonal matrix then $\phi(\pi'M\pi) = \phi(M)$)

(b) $\sum_{i=1}^{p} f(\mu_i) \leq \sum_{i=1}^{p} f(\nu_i)$ if $\mu_i \geq \nu_i$ for all $1 \leq i \leq p$.

(c) if $\mu_1 \leq \mu_2 = \cdots = \mu_p$, $\nu_1 \leq \nu_2 = \cdots = \nu_p$, $\mu_1 \geq \nu_1$, and

$\sum_{i=1}^{p} \mu_i = \sum_{i=1}^{p} \nu_i$ then $\sum_{i=1}^{p} f(\mu_i) \leq \sum_{i=1}^{p} f(\nu_i)$.

Property (a) follows from the fact that $f'' > 0$. Property (b) follows from the fact that $f' < 0$. Property (c) follows from the fact that ϕ regarded as a function of $(\mu_1,\ldots,\mu_p)'$ is Schur convex.

Now suppose δ is as given in the theorem. Let $d \in C(b,k,p)$ be any design which is binary in the test treatments. By (a) and lemma 2.2, $\phi(\bar{M}(d)) \le \phi(M(d))$. If $r_0(d) > bk/2$ by lemma 2.5 there exists $d* \in C(b,k,p)$ with $r_0(d*) < bk/2$ and $\phi(\bar{M}(d*)) \le \phi(\bar{M}(d))$. Replace d by $d*$. If $r_0(d) \le bk/2$ let $d* = d$. Notice by lemma 2.1 $\bar{M}(d*)$ has eigenvalues

$$\mu_1(d*) = (r_0(d*) - \sum_{j=1}^{b} r_{0j}^2(d*)/k)/p$$

$$\mu_2(d*) = \ldots = \mu_p(d*)$$

$$= \{b(k-1)-((k-1)/k)r_0(d*)-(r_0(d*) - \sum_{j=1}^{b} r_{0j}^2(d*)/k)/p\}/(p-1).$$

Using the facts $k \ge 2$, $r_0(d*) \le bk/2$, and some calculus, one can prove that,

$$\mu_2(d*) \ge bk/4p$$

$$= \max(r_0 - \sum_{j=1}^{b} r_{0j}^2/k)/p$$

$$\ge \mu_1(d*)$$

where the maximum is over all real numbers $r_0, r_{01}, \ldots, r_{0j}$ such that $r_0 \ge 0$, $r_{0j} \ge 0$, $1 \le j \le b$, and $\sum_{j=1}^{b} r_{0j} = r_0 \le bk/2$. Thus the eigenvalues $\mu_1(d*), \mu_2(d*), \ldots, \mu_p(d*)$ of $\bar{M}(d*)$ satisfy $u_1(d*) \le u_2(d*) = \ldots = \mu_p(d*)$.

Next notice

(2.7) $\phi(\bar{M}(d*))$

$$= f(u_1(d*)) + (p-1)f(u_2(d*)) = f(\{r_0(d*) - \sum_{j=1}^{b} r_{0j}^2(d*)/k\}/p)$$

$$+ (p-1)f(\{b(k-1)-((k-1)/k)r_0(d*)-(r_0(d*) - \sum_{j=1}^{b} r_{0j}^2(d*)/k)/p\}/(p-1)).$$

For a fixed value of $r_0(d^*) \leq bk/2$ we have $\mu_1(d^*) + (p-1)\mu_2(d^*)$
$= (k-1)(b-r_0(d^*)/k) =$ constant and the largest possible value of $\mu_1(d^*)$

$= (r_0(d^*) - \sum_{j=1}^{b} r_{0j}^2(d^*)/k)/p$ occurs when $b(1+[r_0(d^*)/b])-r_0(d^*)$ of the

$r_{0j}(d^*)$ are $[r_0(d^*)/b]$ and $r_0(d^*) - b[r_0(d^*)/b]$ of the $r_{0j}(d^*)$ are

$[r_0(d^*)/b] + 1$ by lemma 2.4. This choice of the $r_{0j}(d^*)$ maximizes $\mu_1(d^*)$

for fixed $r_0(d^*)$ and hence by property (c) of ϕ minimizes $\phi(\bar{M}(d^*))$. If

we then select a value of $r_0(d^*) \leq bk/2$ (with the optimal choice of the

$r_{0j}(d^*)$) which minimizes the R.H.S. of (2.7) we see that this is precise-

ly the value of $r_0(\delta)$ and the $r_{0j}(\delta)$ stated in the theorem. We thus con-

clude δ is a design minimizing $\phi(\bar{M}(d^*))$ among all d^* which are binary in

test treatments and have $r_0(d^*) \leq bk/2$. Since $M(\delta)$ is completely symmet-

ric, $M(\delta) = \bar{M}(\delta)$ and we see using lemma 2.2 that $\phi(M(\delta)) \leq \phi(\bar{M}(d)) \leq \phi(M(d))$

(d is the design, binary in test treatments, we chose arbitrarily) we con-

clude δ is ϕ-optimal among all d which are binary in test treatments.

Property (b) of ϕ and lemma 2.3 then give us that δ is ϕ-optimal among all

designs.

Theorem 2.1 is useful for finding optimal designs for many ϕ such

as $\phi(M) = \sum_{i=1}^{p} - \ln\mu_i$ (D-optimality) and $\phi(M) = \sum_{i=1}^{p} 1/\mu_i$ (A-optimality).

It is not directly applicable to the problem of finding E-optimal designs,

i.e. the design $\delta \in C(b,k,p)$ which minimizes the maximum eigenvalue of

$M^{-1}(\delta)$ (or maximizes the minimum eigenvalue of $M(\delta)$).

As mentioned in the introduction A-optimal designs are statistically

very meaningful. So we examine such designs in some detail. A design

$d \in C(b,k,p)$ is A-optimal if it minimizes $\text{tr } M^{-1}(d)$ over $C(b,k,p)$. In the

notation of theorem 2.1 this means $\phi(M(d)) = \text{tr } M^{-1}(d)$ and $f(\mu) = 1/\mu$.

Equations (2.5) and (2.6) then become

$$(2.7) \qquad g(r;b,k,p) = p/\{r-(h(r;b)/k)\}$$

$$+ (p-1)^2/\{b(k-1)-r(k-1)/k-(r-h(r;b)/k)/p\}$$

with

$$(2.8) \qquad h(r;b) = [r/b]^2(b+b[r/b]-r) + (r-b[r/b])([r/b]+1)^2.$$

The following result result is a consequence of theorem 2.1.

<u>Theorem 2.2.</u>   Suppose R is the value of the integer r, $0 \le r \le [bk/2]$, which minimizes $g(r;b,k,p)$ as given in (2.7). Also suppose $\delta \in C(b,k,p)$ is a B.T.I.B. design such that

(i) δ is binary in test treatments

(ii) $r_0(\delta) = R$

(iii) $r_{0j}(\delta) = [R/b]$ or $[R/b] + 1$ for $1 \le j \le p$

then δ is A-optimal over $C(b,k,p)$.

The integer r which minimizes $g(r;b,k,p)$ can easily be found using a computer. As an example, $r = 18$ minimizes $g(r;24,3,9)$ and the following B.T.I.B. design is therefore A-optimal.

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 2 & 3 & 4 & 5 \\ 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 4 & 4 & 5 & 6 & 6 & 7 & 7 & 2 & 6 & 3 & 4 & 5 & 8 \\ 3 & 4 & 5 & 8 & 4 & 5 & 7 & 8 & 5 & 7 & 9 & 6 & 9 & 6 & 8 & 9 & 8 & 9 & 9 & 7 & 6 & 8 & 7 & 9 \end{pmatrix}$$

Here columns correspond to blocks and the numbers are the treatment labels.

Having determined the integer R, the next step is to investigate whether a B.T.I.B. design satisfying (i)-(iii) exists or not. Writing $q = [R/b]$ and $a = R - bq$, an A-optimal design looks like

$$d = \begin{pmatrix} d_{(1)} \\ d_{(2)} \end{pmatrix},$$

where $d_{(1)}$ consists of q plots in each of b blocks and $d_{(2)}$ the rest of the $k - q$ plots in the blocks. $d_{(1)}$ consists entirely of the control, while $d_{(2)}$ is binary in all $p + 1$ treatments with the control appearing a times.

The A-optimal design shown above gives an example of $d = d_{(2)}$ since here $q = 0$.

If $a = 0$, then $d_{(2)}$ has to be a B.I.B. design in the p test treatments. The following table gives some examples of A-optimal designs having this structure.

b	k	b	q
10	3	5	1
14	4	7	1
30	2	4	1
30	4	5	1
30	4	6	1
30	5	10	1
30	6	25	1

Let us denote by d_q a design in $C(b,k,p)$ which is a B.I.B. in the $k - q$ plots of b blocks in the p test treatments, augmented by the control in each of the remaining q plots of b blocks. Designs of this type have been mentioned briefly by Cox (1958, p. 238); Pešek (1974) has look at d_1. Neither of them have considered these as optimal designs. The interested reader may find their efforts put in perspective in Bechhofer and Tamhane (1981). We shall now show that for many q, d_q cannot be a very bad design - it is at least A - better than a B.I.B. design in all $p + 1$ treatments.

A B.I.B. design is a binary B.T.I.B. design with $r_0(d) = bk/(p+1)$. Moreover, for any B.T.I.B. design, tr $M(d)^{-1} = g(r_0(d);b,k,p)$. Hence we look at the sign of the function,

(2.9) $g_1(q) \equiv g(qb;b,k,p) - g(bk/(p+1);b,k,p)$

$$= p/\{r-(bq^2)/k\}$$

$$+ (p-1)^2/\{b(k-1)-r(k-1)/k-(r-(bq^2)/k)/p\} - 2p^2/\{b(k-1)\} ,$$

with q allowed to be positive integers only. If one allows q to be any

real number, then it is easy to see that the polynomial equation

$$g_1(q) = 0$$

has no roots in the interval $[1,(k-1)/2]$ of q. Moreover $g_1(1) < 0$ and $g_1((k-1)/2) < 0$, but $g_1(k/2) > 0$. Thus in particular $g_1(q) < 0$, q = 1,2, ...,$[(k-1)/2]$. We summarize this in the following theorem.

Theorem 2.3. d_q is A-better than a B.I.B. design in all p + 1 treatments for all q = 1,2,...,$[(k-1)/2]$, whenever they exist.

3. E-Optimal Designs

We now determine E-optimal designs.

Theorem 3.1.   If there exists $\delta \in C(b,k,p)$ such that

   (i)   every block contains exactly k/2 replications of the control, if k is even, or either $[k/2]$ or $[k/2] + 1$ replications of the control if k is odd

and

   (ii) $\lambda_{01}(\delta) = \lambda_{02}(\delta) = \ldots = \lambda_{0p}(\delta)$

then δ is E-optimal over $C(b,k,p)$.

pf.   We first show that $\lambda_{01}(\delta)/k$ is the minimum eigenvalue of $M(\delta)$. To see this, notice that the sum of the entires in the i-th row of $M(\delta)$ is $\lambda_{0i}(\delta)/k$. Since $\lambda_{01}(\delta) = \lambda_{0i}(\delta)$ for all i, all the row sums of $M(\delta)$ are $\lambda_{01}(\delta)/k$. It therefore follows that the p × 1 vector $(1,1,\ldots,1)'$ is an eigenvector of $M(\delta)$ with eigenvalue $\lambda_{01}(\delta)/k$.

To verify that $\lambda_{01}(\delta)/k$ is the smallest eigenvalue of $M(\delta)$, let $\vec{e}$ be any eigenvector of $M(\delta)$ other than $(1,\ldots,1)'$. Without loss of generality we may assume the largest coordinate in absolute value of $\vec{e}$ is +1. Suppose +1 is the i-th coordinate of $\vec{e}$. Let λ denote the eigenvalue

of $M(\delta)$ corresponding to the eigenvector $\vec{e}$. Let e_j denote the j-th coordinate of $\vec{e}$ and $m_{ij}(\delta)$ the i,j-th entry of $M(\delta)$. The i-th coordinate of $M(\delta)\ \vec{e}$ is

$$\sum_{j=1}^{p} m_{ij}(\delta)e_j = e_i m_{ii}(\delta) + \sum_{\substack{j=1 \\ j\neq i}}^{p} e_j m_{ij}(\delta) \geq m_{ii}(\delta) + \sum_{\substack{j=1 \\ j\neq i}}^{p} m_{ij}(\delta)$$

$$= \sum_{j=1}^{p} m_{ij}(\delta) = \lambda_{0i}(\delta)/k = \lambda_{01}(\delta)/k.$$

The inequalities above follow from the fact that $e_i = +1$, $|e_j| \leq 1$ for all j, and $m_{ij}(\delta) \leq 0$ for $i \neq j$. Since $\lambda\vec{e} = M(\delta)\vec{e}$ and the i-th coordinate of $\lambda\vec{e}$ is $\lambda e_i = \lambda$, we have $\lambda \geq \lambda_{01}(\delta)/k$.

Since $\vec{e}$ was an arbitrary eigenvector, hence λ was an arbitrary eigenvalue, we conclude $\lambda_{01}(\delta)/k$ is the minimum eigenvalue of $M(\delta)$.

Notice

$$\lambda_{01}(\delta)/k = \{ \sum_{i=1}^{p} \lambda_{0i}(\delta)/k \}/p = \{r_0(\delta) - \sum_{j=1}^{b} r_{0j}^2(\delta)/k\}/p .$$

By a proof similar to that used in lemma 2.4 one can show that among all integers $r_{01}, r_{02}, \ldots, r_{0b}$ such that $0 \leq r_{0j} \leq k$, the value of

$r_0 - \sum_{j=1}^{b} r_{0j}^2/k(r_0 = \sum_{j=1}^{b} r_{0j})$ is maximized by choosing all $r_{0j} = k/2$ if k is even or $r_{0j} = [k/2]$ or $[k/2] + 1$, $j = 1, \ldots, b$, if k is odd. Since these are precisely the values of the $r_{0j}(\delta)$ we conclude

(3.1)   min eigenvalue of $M(\delta) = (r_0(\delta) - \sum_{j=1}^{b} r_{0j}^2(\delta)/k)/p$

$$\geq (r_0(d) - \sum_{j=1}^{b} r_{0j}^2(d)/k)/p$$

for all $d \in C(b,k,p)$. For any $d \in C(b,k,p)$

$$\text{min eigenvalue of } M(d) = \min_{||\vec{u}||=1} \vec{u}'M(d)\vec{u}$$

$$\leq (1,1,\ldots,1)M(d)(1,1,\ldots,1)'/p$$

$$= \sum_{i=1}^{p} \sum_{j=1}^{p} m_{ij}(d)/p = \sum_{i=1}^{p} \lambda_{0i}(d)/kp$$

$$\leq \text{min eigenvalue of } M(\delta)$$

where we have used the facts that $\sum_{j=1}^{p} m_{ij}(d) = \lambda_{0i}(d)/k$,

$\sum_{i=1}^{p} \lambda_{0i}(d)/k = r_0(d) - \frac{1}{k} \sum_{j=1}^{b} r_{0j}^2(d)$, and (3.1).

We conclude that δ has the largest minimum eigenvalue among all $d \in C(b,k,p)$ and hence it follows that δ is E-optimal over $C(b,k,p)$.

Theorem 3.1 can be used to find E-optimal designs for comparing test treatments to a control. When k is even each block in an E-optimal design d must have exactly $k/2$ replications of the control. It is straightforward to see that a necessary and sufficient condition for a design d to be E-optimal when k is even is that $m = bk/2p$ be an integer, $r_i(d) = m$ for all $1 \leq i \leq p$, and each block contain exactly $k/2$ replications of the control. Thus each of the following designs are E-optimal when $b = k = p = 4$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 3 & 3 \\ 2 & 2 & 4 & 4 \end{pmatrix}.$$

When k is odd there is more flexibility in finding designs which are E-optimal. In particular an E-optimal design d can have either [k/2] or [k/2] + 1 replications of the control in a given block and this flexibility allows one to meet the condition $\lambda_{01}(d) = \ldots = \lambda_{0p}(d)$ more easily than when k is even. For example, when $b = 5$, $k = 5$, and $p = 6$ it is easy

to check that the condition $\lambda_{01}(d) = \ldots = \lambda_{06}(d)$ cannot be met if all blocks have exactly 2 replications of the control or if all blocks have exactly three replications of the control. However the design

$$d = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 4 & 0 & 0 & 0 \\ 2 & 5 & 1 & 3 & 5 \\ 3 & 6 & 2 & 4 & 6 \end{pmatrix}$$

has $\lambda_{0i}(d) = 5$ for all $1 \leq i \leq 6$ and is E-optimal.

One can show that when k is odd if $b = \gamma + \omega$, where α and β are integers ≥ 0 such that $s = \gamma[k/2]/p$ and $t = \omega([k/2]+1)/p$ are both non-negative integers, then an E-optimal design d exists. In fact any design consisting of γ blocks in which each test treatment appears exactly s times and the control appears exactly $[k/2] + 1$ times in each of the γ blocks, and consisting of ω blocks in which each test treatment appears exactly t times and the control appears exactly $[k/2]$ times in each of the ω blocks, is E-optimal.

It should also be remarked that if an E-optimal design also happens to be a B.T.I.B. which is binary in test treatments, then the design may have additional optimality properties. For example, the design

$$d = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 2 \\ 2 & 3 & 3 \end{pmatrix}$$

with $b = 3$, $k = 3$, $p = 3$ turns out to be both E-optimal and A-optimal.

Even though E-optimality is an effective way of minimizing a norm of $M(d)^{-1}$, in the present context it does not seem to possess a very natural statistical meaning. If one favours a minimax style approach then possibly one way is to minimize the maximum variance of $(\hat{\alpha}_0 - \hat{\alpha}_i)$, the maximum being over $1 \leq i \leq p$, minimum over all $d \in C(b,k,p)$. In other words, one considers

the criterion $\phi(M(d))$ = maximum diagonal entry of $M^{-1}(d)$. Since ϕ is convex and permutation invariant lemma 2.2 says that $\phi(\bar{M}(d)) \leq \phi(M(d))$ for any $d \in C(b,k,p)$. Furthermore, since $\bar{M}(d)$ is completely symmetric, it is easily verified that $\phi(\bar{M}(d)) = \text{tr } \bar{M}(d)^{-1}/p$. From these two observations it follows that if $\delta \in C(b,k,p)$ is as in theorem 2.2 than it is ϕ-optimal as well as A-optimal. This lends additional significance to the A-optimal designs.

A class of criteria that are sometimes considered in optimal design investigations (see Kiefer (1974)) are the ϕ_q criteria, $0 < q < \infty$, where

$$\phi_q(M(d)) = \sum_{i=1}^{p} \mu_i^{-q}$$

and $\mu_1 \leq \ldots \leq \mu_p$ are the eigenvalues of $M(d)$. D-optimality and E-optimality are limiting cases of these criteria in the sense that $\lim_{q \to 0}(\phi_q(M(d))/p)^{1/q}$ $= (\det M^{-1}(d))^{1/p}$ and $\lim_{q \to \infty}(\phi_q(M(d))/p)^{1/q} = $ max eigenvalue of $M^{-1}(d)$. In particular, ϕ_0 and ϕ_∞ are sometimes used to denote the D-optimality and E-optimality criteria, respectively. Also notice that ϕ_1 is just the A-optimality criterion.

An examination of our above results for D-, A-, and E-optimality (or for ϕ_0, ϕ_1, and ϕ_∞) indicates that the number of replications of the control in an optimal design is smallest for D-optimality, second smallest for A-optimality, and largest for E-optimality. This suggests that the number of replications of the control in a B.T.I.B. design which is ϕ_q-optimal is increasing as q increases. Since ϕ_q, $0 < q < \infty$, satisfies the conditions of theorem 2.1, it is possible (although somewhat tedious) to verify that this is indeed the case. From this it follows that if $d \in C(b,k,p)$ is a B.T.I.B. design which is binary in test treatments with

$[bk/(p+1)] < r_0(d) < b[k/2]$, then d is ϕ_q-optimal for some $0 < q < \infty$.

4. Concluding Remarks

B.T.I.B. designs were introduced by Bechhofer and Tamhane (1981). The property of being balanced in test treatments make these designs attractive for use in comparing test treatments to a control. It has been an open question as to what sort of optimality properties, if any, these designs might have. This paper answers that question in part by showing that certain B.T.I.B. designs do indeed have some optimal properties. It is hoped that this paper will provide added incentive for the study of these designs, particularly their construction.

One interesting feature of the results contained in this paper is that exactly what design is optimal depends very mcuh on the optimality criterion used. This is different from the usual incomplete block design setting where orthonormal treatment contrasts are of interest. In that setting optimal designs are often found to be somewhat independent of the criterion used and hence selection of an appropriate design is simplified. The results of this paper show that the selection of an appropriate design for comparing test treatments with a control is unfortunately sensitive to the optimality criterion used. Unless one has a clear idea of the optimality criterion one wishes to use in selecting a design, selection of an appropriate design is not as straightforward as in the traditional setting of estimating an orthonormal basis of treatment contrasts. We do recognize, however, the poignant statistical appeal of A-optimality.

REFERENCES

1. Bechhofer, R. E. and Tamhane, A. C. (1981). Incomplete block designs for comparing treatments with a control: General theory. Technometrics, 23, 45-57.

2. Cheng, C. S. and Wu, C. F. (1980). Balanced Repeated Measurements Designs. Ann. Statist., 8, 1272-1283.

3. Cox , D. R. (1958). Planning of Experiments, New York, John Wiley and Sons.

4. Hedayat, A. S. (1974). Lecture Notes on Optimal Experiments (unpublished.)

5. Kiefer, J. (1958). On the nonrandomized optimality and randomized nonoptimality of symmetrical designs. Ann. Math. Statist., 29, 475-699.

6. Kiefer, J. (1959). Optimum experimental designs. J. Roy. Statist. Soc. Ser. B, 21, 272-319.

7. Kiefer, J. (1971). The role of symmetry and approximation in exact design optimality. In Statistical Decision Theory and Related Topics (S. S. Gupta and J. Yackel, eds.), Academic Press, New York, 109-118.

8. Kiefer, J. (1974). General equivalence theory for optimum designs (approximate theory). Ann. Statist. 2, 849-879.

9. Kiefer, J. (1975). Construction and Optimality of Generalized Youden Designs. A Survey of Statistical Design and Linear Models (J. Srivastava ed.) North Holland, New York, 333-353.

10. Pesek, J. (1974). The Efficiency of Controls in Balanced Incomplete Block Designs, Biometrische Zeitschrift, 16, 21-26.

<u>pf.</u>   In each block of M(d) replace any duplicates of test treatments by test treatments not in the block so that each block is binary in test treatments (this is possible since $k \leq p$). Call the resulting design d*. Notice d* is binary in test treatments, has $r_{0j}(d^*) = r_{0j}(d)$ for all $1 \leq j \leq b$, and has $\sum_{i=1}^{p} r_i(d^*) = \sum_{i=1}^{p} r_i(d)$. As a result it is easy to see

$$\sum_{i=1}^{p} \sum_{j=1}^{b} r_{ij}^2(d^*) \leq \sum_{i=1}^{p} \sum_{j=1}^{b} r_{ij}^2(d).$$

From lemma 2.1 it then follows that the eigenvalues of $\bar{M}(d)$ and $\bar{M}(d^*)$ satisfy $\mu_1(d) = \mu_1(d^*)$ and $\mu_2(d) = \ldots = \mu_p(d) \leq \mu_2(d^*) = \ldots = \mu_p(d^*)$. Hence by the property of ϕ given in the statement of the lemma, $\phi(\bar{M}(d^*)) \leq \phi(\bar{M}(d))$.

END

FILMED